

Chloroform

67-66-3 | DTXSID1020306

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.87            | 0.81 | 0.87           | 0.82 | 0.86       | 0.86 |

Model Results

Predicted value: 4.85e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.33e-01

Confidence level: 8.44e-01

Nearest Neighbors from the Training Set

|  |   |   |
|--|---|---|
| <div>Image not found</div> <div>Chloroform</div> <div>Measured: 6.66e-02</div> <div>Predicted: 4.85e-02</div>            | <div>Image not found</div> <div>Bromodichloromethane</div> <div>Measured: 1.85e-02</div> <div>Predicted: 2.19e-02</div>     | <div>Image not found</div> <div>1,1-Dichloroethane</div> <div>Measured: 5.11e-02</div> <div>Predicted: 4.60e-02</div>       |
| <div>Image not found</div> <div>1,1,2-Trichloroethane</div> <div>Measured: 3.31e-02</div> <div>Predicted: 2.84e-02</div> | <div>Image not found</div> <div>(Z)-1,2-Dichloroethylene</div> <div>Measured: 4.84e-02</div> <div>Predicted: 4.42e-02</div> | <div>Image not found</div> <div>(E)-1,2-Dichloroethylene</div> <div>Measured: 4.84e-02</div> <div>Predicted: 4.42e-02</div> |